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Understanding the effect of fluoroethylene carbonate addition into an electrolyte - a molecular dynamics study

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Abstract

Fluoroethylene carbonate (FEC) is used as an electrolyte additive of Li-ion rechargeable batteries to mitigate volume expansion of the anode during battery cycling. However, the effect of FEC addition on the electrolyte has not been studied adequately. Here we report molecular dynamics simulations of electrolyte mixtures commonly used in Li-ion batteries while focusing on the effect that varying FEC concentration has on the transport and solvation properties of other electrolyte components. Here, bonded and non-bonded force field parameters for the ethylene carbonate (EC), dimethyl carbonate (DMC) and FEC molecules were assigned using the Generalized Amber Force Field (GAFF) through Moltemplate. All the simulations were conducted using Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code. The systems were allowed to evolve for 2 ns first from their initial configuration. Once it was done, the simulations were further run for 30 ns. After this, 5 ns production runs were performed to collect the positions of atoms. The results showed that FEC addition, even as a minor component, has significantly affected the diffusion constants of species and total ionic conductivity of the electrolyte compared to those without addition. Moreover, the lithium ions show a lower rate of diffusion compared to hexafluorophosphate ions irrespective of FEC addition. Upon the addition of 10 % FEC, both lithium ions and hexafluorophosphate ions show a small increase in rate of diffusion. However, further addition has again decreased the diffusion of lithium ions. Further, Solvent species of ethylene carbonate and fluoroethylene carbonate show higher diffusion rate compared to lithium ions and hexafluorophosphate ions. Finally, these findings reveal that addition of FEC has changed the transportation and clustering properties of the EC/DMC/lithium hexafluorophosphate system.

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